

# Lattice Boltzmann Scheme associated with flexible Prandtl number and specific heat ratio based on the polyatomic ES-BGK model

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A lattice Boltzmann scheme associated with flexible Prandtl number and specific heat ratio is proposed, which is based on the polyatomic ellipsoidal statistics model(ES-BGK). The Prandtl number can be modified by a parameter of the Gaussian distribution and the specific heat ratio can be modified by additional free degrees. For the sake of constructing the scheme proposed, the Gaussian distribution is expanded on the Hermite polynomials and the general term formula for the Hermite coefficients of the Gaussian distribution is deduced. Benchmarks are carried out to verify the scheme proposed. The numerical results are in good agreement with the analytical solutions.

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## I. INTRODUCTION

In recent 20 years, the lattice Boltzmann method (LBM) is widely applied to a variety of complex flows, such as multiphase and multicomponent fluids[1][2], fluid flows through porous media[3], turbulence[4], magnetohydrodynamics and so on. Nevertheless, when the LBM is applied to thermal fluids, there are some unresolved problems. Although the Navier-Stokes equations(including the energy conversation equation) can be derived from the evolution equation via the Chapman-Enskog expansion, the specific heat ratio and the Prandtl number is fixed. In other word, these physical performances of fluids are not realistic.

To overcome the drawback pointed above, some lattice Boltzmann schemes associated with flexible specific heat ratio or Prandtl number have been proposed. In order to modify the specific heat ratio, new variables such as rotational velocity or rotational internal energy are introduced and discretized in the velocity space[5–8]. For the sake of modifying the Prandtl number, a quasi-equilibrium or other similar item which control the Prandtl number is introduced[9–12]. These lattice Boltzmann schemes associated with flexible Prandtl number are based on the BGK model.

Other than the BGK, the ellipsoidal statistics model(ES-BGK) is also popular in kinetics, in which the Maxwell-Boltzmann distribution is replaced by the Gaussian distribution. The ES-BGK model is first proposed by Holway Jr in 1965[13]. In recent years, the ES-BGK model attracts new attention partly because P.Andrie

verified that the model satisfies the entropy inequality for the range  $\frac{2}{3} \leq Pr \leq 1$ [14–16]. The ES-BGK model for polyatomic gases is also discussed[17]. The polyatomic ES-BGK model gives the proper transport coefficients in the hydrodynamic limit for the polyatomic gases. That means not only the Prandtl number but also the specific haet ratio are adjustable.

The polyatomic ES model is applied to the LBM in this work. A Lattice Boltzmann scheme with flexible Prandtl number and specific heat ratio is proposed. The general term formula for the Hermite coefficients of the Gaussian distribution is deduced. This is the key point of the lattice Boltzmann scheme propose by this work. Employing the general term formula of the Hermite coefficient of the Gaussian distribution, we can easily deduce high order terms of the Hermite coefficients of the Gaussian distribution. It make it easy to construct high order lattice Boltzmann schemes based on the ES-BGK model.

## II. POLYATOMIC ES-BGK MODEL

In this section, we discuss the polyatomic ES-BGK model. We begin with the kinetic equation of the polyatomic distribution function  $f(\xi, \mathbf{x}, t, I)$ [14][17]

$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial \mathbf{x}} = \Omega, \quad (1)$$

where  $f(\xi, \mathbf{x}, I, t)$  is the distribution function with the particle velocity  $\xi$  and the internal energy  $\epsilon = I^{\frac{2}{N_f}}$  at position  $\mathbf{x}$  and time  $t$ ,  $N_f$  is the additional degrees of freedom of the gas and  $\Omega(f)$  is the collision operator

$$\Omega(f) = -\frac{1}{\tau(1 - \nu + \nu\kappa)}(f - G[f]). \quad (2)$$

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Here  $\tau$  is the relaxation time,  $G[f]$  is the polyatomic Gaussian model, the parameter  $-\frac{2}{3} \leq \nu < 1$  and  $0 \leq \kappa \leq 1$  are introduced to modify the Prandtl number and the specific heat ratio.

The density  $\rho$ , macroscopic velocity  $\mathbf{u}$ , and the total energy  $E$ , the specific internal energy  $e$  are defined by the moments of the distribution function  $f$

$$\rho = \int_{R^D} \int_{R^+} f d\boldsymbol{\xi} dI, \quad (3a)$$

$$\rho \mathbf{u} = \int_{R^D} \int_{R^+} \boldsymbol{\xi} f d\boldsymbol{\xi} dI, \quad (3b)$$

$$E = \frac{1}{2} \rho u^2 + \rho e = \int_{R^D} \int_{R^+} \left( \frac{1}{2} \xi^2 + I^{\frac{2}{N_f}} \right) f d\boldsymbol{\xi} dI. \quad (3c)$$

Here  $D$  is the space dimension.

The specific internal energy  $e$  can be divided into two part, i.e. the internal energy of translational velocity  $e_{tr}$  and the energy associated with the internal structure  $e_{int}$

$$e = e_{tr} + e_{int}, \quad (4)$$

where

$$e_{tr} = \frac{1}{\rho} \int_{R^D} \int_{R^+} \frac{1}{2} (\boldsymbol{\xi} - \mathbf{u})^2 f d\boldsymbol{\xi} dI, \quad (5)$$

$$e_{int} = \frac{1}{\rho} \int_{R^D} \int_{R^+} I^{2/N_f} f d\boldsymbol{\xi} dI. \quad (6)$$

The relationship between temperature  $T$ ,  $T_{tr}$ ,  $T_{int}$  and the corresponding energy  $e$ ,  $e_{tr}$ ,  $e_{int}$  are

$$e = \frac{D + N_f}{2} R_g T_{eq}, \quad e_{tr} = \frac{D}{2} R_g T_{tr}, \quad e_{int} = \frac{N_f}{2} R_g T_{int}. \quad (7)$$

Here  $R_g$  is the general gas constant.

The state equation is  $p = \rho R_g T_{eq}$ . Here  $p$  is the pressure.

The generalized Gaussian model is defined by

$$G[f] = \frac{\Lambda_{N_f} \rho}{\sqrt{\det(2\pi\boldsymbol{\Lambda})}} \frac{1}{R_g T_{rel}^{N_f/2}} \times \exp \left[ -\frac{1}{2} (\boldsymbol{\xi} - \mathbf{u}) \cdot \boldsymbol{\Lambda}^{-1} \cdot (\boldsymbol{\xi} - \mathbf{u}) - \frac{I^{\frac{2}{N_f}}}{R_g T_{rel}} \right]. \quad (8)$$

Here  $\boldsymbol{\Lambda}$  is the corrected tensor

$$\boldsymbol{\Lambda} = (1 - \kappa) [(1 - \nu) R_g T_{tr} \boldsymbol{\delta} + \nu \boldsymbol{\sigma}] + \kappa R_g T_{eq} \boldsymbol{\delta}. \quad (9)$$

Here  $\boldsymbol{\sigma}$  is the opposite stress tensor

$$\boldsymbol{\sigma} = \frac{1}{\rho} \int (\boldsymbol{\xi} - \mathbf{u})(\boldsymbol{\xi} - \mathbf{u}) f d\boldsymbol{\xi}. \quad (10)$$

and  $\boldsymbol{\delta}$  is the unit tensor. The relaxation temperature  $T_{rel}$  is defined by

$$T_{rel} = \kappa T_{eq} + (1 - \kappa) T_{int}. \quad (11)$$

The constant  $\Lambda_\delta$  is defined by

$$\Lambda_{N_f}^{-1} = \int e^{-I^{2/N_f}} dI. \quad (12)$$

### III. POLYATOMIC ES-BGK MODEL: DESCRIPTION WITH TWO DISTRIBUTION FUNCTIONS

The evolution equation of the polyatomic distribution function  $f(\boldsymbol{\xi}, \mathbf{x}, t, I)$  is

$$\frac{\partial}{\partial t} f + \boldsymbol{\xi} \cdot \frac{\partial}{\partial \mathbf{x}} f = -\frac{1}{\tau(1 - \nu + \kappa\nu)} (f - G[f]). \quad (13)$$

This kinetic equation can be reduced to two distribution function, i.e. the distribution function of mass  $g(\boldsymbol{\xi})$  and that of energy  $h(\boldsymbol{\xi})$ . This idea is proposed by C.K.Chu[18][19] and V.A.Rykov[20]. Their main aim is to save computational resource. When the idea is applied to the LBM, there is another advantage that it is not necessary to discretize  $\epsilon$  on lattices. The lattices employed in the scheme proposed by this work are DnQb models. These lattice models are easier to be constructed than the ones in which both the translational velocity of particle and the new introduced parameter are discretized [6, 7, 11, 21].

The distribution of  $g(\boldsymbol{\xi}, \mathbf{x}, t)$  and  $h(\boldsymbol{\xi}, \mathbf{x}, t)$  are defined by

$$g(\boldsymbol{\xi}, \mathbf{x}, t) = \int_{R^+} f(\boldsymbol{\xi}, I, \mathbf{x}, t) dI, \quad (14a)$$

$$h(\boldsymbol{\xi}, \mathbf{x}, t) = \int_{R^+} I^{\frac{2}{N_f}} f(\boldsymbol{\xi}, I, \mathbf{x}, t) dI. \quad (14b)$$

The macroscopic quantities are defined by the moments of the distribution function of mass  $g(\boldsymbol{\xi})$  and that of the energy  $h(\boldsymbol{\xi})$

$$\rho = \int_{R^D} g(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (15a)$$

$$\rho \mathbf{u} = \int_{R^D} \boldsymbol{\xi} g(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (15b)$$

$$\rho E = \int_{R^D} \left[ \frac{1}{2} \xi^2 g(\boldsymbol{\xi}) + h(\boldsymbol{\xi}) \right] d\boldsymbol{\xi}. \quad (15c)$$

Integrating Eq(13) on  $I$ , we obtain the evolution equation of  $g(\boldsymbol{\xi})$

$$\frac{\partial}{\partial t} g + \boldsymbol{\xi} \cdot \nabla g = -\frac{1}{\tau(1 - \nu + \kappa\nu)} (g - G[g, h]). \quad (16)$$

Here  $G[g, h]$  is

$$G[g, h] = \frac{\rho}{\sqrt{\det(2\pi\boldsymbol{\Lambda})}} \exp \left[ -\frac{1}{2} (\boldsymbol{\xi} - \mathbf{u}) \cdot \boldsymbol{\Lambda}^{-1} \cdot (\boldsymbol{\xi} - \mathbf{u}) \right]. \quad (17)$$

Integrating Eq(13)  $\times I^{\frac{2}{N_f}}$  on  $I$ , we obtain the evolution equation of  $h(\boldsymbol{\xi})$

$$\frac{\partial}{\partial t} h + \boldsymbol{\xi} \cdot \nabla h = -\frac{1}{\tau(1 - \nu + \kappa\nu)} \left( h - \frac{N_f}{2} R_g T_{rel} G[g, h] \right). \quad (18)$$

From Eq(16) and (18), the Navier-Stokes equations associated with flexible specific heat ratio and Prandtl number can be derived via the Chapman-Enskog expansion[14][22]. In the derived Navier-Stokes equations, the viscosity tensor is

$$\boldsymbol{\sigma} = \mu(\nabla \mathbf{u} + \mathbf{u} \nabla - \alpha \nabla \cdot \mathbf{u} \boldsymbol{\delta}).$$

Here  $\mu = \tau p / (1 - \nu + \kappa \nu)$  is the viscosity coefficient and  $\mu \alpha$  is the second viscosity coefficient, where

$$\alpha = (\gamma - 1) - \frac{1 - \kappa}{\kappa} (1 - \nu) \left( \frac{D + 2}{D} - \gamma \right). \quad (19)$$

The specific heat ratio and the Prandtl number  $Pr$  in the recovered Navier-Stokes equation are defined by

$$\gamma = \frac{N_f + D + 2}{N_f + D}, \quad (20)$$

$$\frac{2}{3} \leq Pr = \frac{1}{1 - \nu + \kappa \nu} < +\infty. \quad (21)$$

#### IV. THE GENERAL TERM FORMULA FOR THE HERMITE COEFFICIENTS OF THE GAUSSIAN DISTRIBUTION

The expansion of the Maxwell-Boltzmann distribution on the Hermite polynomial has been discussed [23–25]. Here, we expand the Gaussian distribution on the Hermite polynomials. This is the key point of constructing the lattice Boltzmann scheme based on the ES-BGK model.

Three identities given by Grad i.e. Eq(4),(12) and (16) of [23] will be employed in the following paragraphs,

$$(\mathbf{x} + \mathbf{y})^n = \sum_{r=0}^n \mathbf{x}^r \mathbf{y}^{n-r}, \quad (22)$$

$$\mu_{2n} = \int \omega(\mathbf{x}) \mathbf{x}^{2n} d\mathbf{x} = \boldsymbol{\delta}^n, \quad (23)$$

$$\begin{aligned} \mathbf{H}^{(n)} &= \mathbf{x}^n - \boldsymbol{\delta} \mathbf{x}^{n-2} + \boldsymbol{\delta}^2 \mathbf{x}^{n-4} + \dots, \\ &= (\mathbf{x} - \boldsymbol{\delta})^n, \end{aligned} \quad (24)$$

where  $\mathbf{H}^{(n)}$  is the Hermite polynomials and  $\omega(\mathbf{x})$  is the weight function

$$\omega(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^{D/2}}} \exp\left(-\frac{\mathbf{x}^2}{2}\right).$$

Here, the Grad notes are employed.

The Gaussian distribution  $G$  can be expanded on the Hermite polynomial

$$G = \rho \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}^{(n)} \cdot \mathbf{H}^{(n)}(\boldsymbol{\xi}), \quad (25)$$

where

$$\mathbf{a}^{(n)} = \frac{1}{\rho} \int \mathbf{H}^{(n)}(\boldsymbol{\xi}) G d\boldsymbol{\xi}. \quad (26)$$

Defining

$$(\boldsymbol{\xi} - \mathbf{u}) \cdot \boldsymbol{\Lambda}^{-\frac{1}{2}} = \boldsymbol{\eta}, \quad (27)$$

then we obtain

$$\boldsymbol{\xi} = \mathbf{u} + \boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}} \quad (28)$$

Inserting Eq(28) and (17) into Eq(26), we obtain

$$\begin{aligned} \mathbf{a}^{(n)} &= \frac{1}{\rho} \int \mathbf{H}^{(n)}(\mathbf{u} + \boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}}) \frac{\rho}{\sqrt{\det(2\pi \boldsymbol{\Lambda})}} \\ &\quad \times \exp\left[-\frac{1}{2}(\boldsymbol{\xi} - \mathbf{u}) \cdot \boldsymbol{\Lambda}^{-1} \cdot (\boldsymbol{\xi} - \mathbf{u})\right] d(\mathbf{u} + \boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}}) \\ &= \int \mathbf{H}^{(n)}(\mathbf{u} + \boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}}) \omega(\boldsymbol{\eta}) d\boldsymbol{\eta} \\ &= \sum_{\alpha=0}^{[n/2]} (-1)^\alpha \int \omega(\boldsymbol{\eta}) (\mathbf{u} + \boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}})^{n-2\alpha} \boldsymbol{\delta}^\alpha d\boldsymbol{\eta} \\ &= \sum_{\alpha=0}^{[n/2]} \sum_{\beta=0}^{[n/2]-\alpha} (-1)^\alpha \int \omega(\boldsymbol{\eta}) \mathbf{u}^{n-2(\alpha+\beta)} (\boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^{\frac{1}{2}})^{2\beta} \boldsymbol{\delta}^\alpha d\boldsymbol{\eta} \\ &= \sum_{\alpha=0}^{[n/2]} \sum_{\beta=0}^{[n/2]-\alpha} (-1)^\alpha \mathbf{u}^{n-2(\alpha+\beta)} \boldsymbol{\delta}^\alpha \left[ \int \omega(\boldsymbol{\eta}) \boldsymbol{\eta}^{2\beta} d\boldsymbol{\eta} \cdot \boldsymbol{\Lambda}^\beta \right] \\ &= \sum_{\alpha=0}^{[n/2]} \sum_{\beta=0}^{[n/2]-\alpha} (-1)^\alpha \boldsymbol{\delta}^\alpha (\boldsymbol{\delta}^\beta \cdot \boldsymbol{\Lambda}^\beta) \mathbf{u}^{n-2(\alpha+\beta)} \\ &= \sum_{\alpha=0}^{[n/2]} \sum_{\beta=0}^{[n/2]-\alpha} (-1)^\alpha \boldsymbol{\delta}^\alpha \boldsymbol{\Lambda}^\beta \mathbf{u}^{n-2(\alpha+\beta)}. \end{aligned} \quad (29)$$

Defining  $\chi = \alpha + \beta$ , inserting  $\chi$  into Eq(29) and changing the ranges of the superscripts we obtain

$$\begin{aligned} \mathbf{a}^{(n)} &= \sum_{\chi=0}^{[n/2]} \sum_{\beta=0}^{\chi} (-1)^\beta \boldsymbol{\Lambda}^\beta \boldsymbol{\delta}^{\chi-\beta} \mathbf{u}^{n-2\chi} \\ &= \sum_{\chi=0}^{[n/2]} (\boldsymbol{\Lambda} - \boldsymbol{\delta})^\chi \mathbf{u}^{n-2\chi} \\ &= \sum_{\alpha=0}^{[n/2]} (\boldsymbol{\Lambda} - \boldsymbol{\delta})^\alpha \mathbf{u}^{n-2\alpha}. \end{aligned}$$

Finally, we get

$$\mathbf{a}^{(n)} = \sum_{\alpha=0}^{[n/2]} \sum_{\beta=0}^{\alpha} (-1)^{\alpha-\beta} \boldsymbol{\Lambda}^\beta \boldsymbol{\delta}^{\alpha-\beta} \mathbf{u}^{n-2\alpha}. \quad (30)$$

Eq(30) is the general term formula for the Hermite coefficients of the Gaussian distribution  $G$ . The first sixth

order of  $\mathbf{a}^{(n)}$  is

$$\begin{aligned}
\mathbf{a}^{(0)} &= 1, \\
\mathbf{a}^{(1)} &= \mathbf{u}, \\
\mathbf{a}^{(2)} &= \mathbf{\Lambda} - \boldsymbol{\delta} + \mathbf{u}^2, \\
\mathbf{a}^{(3)} &= (\mathbf{\Lambda} - \boldsymbol{\delta})\mathbf{u} + \mathbf{u}^3, \\
\mathbf{a}^{(4)} &= (\mathbf{\Lambda} - \boldsymbol{\delta})^2 + (\mathbf{\Lambda} - \boldsymbol{\delta})\mathbf{u}^2 + \mathbf{u}^4, \\
\mathbf{a}^{(5)} &= (\mathbf{\Lambda} - \boldsymbol{\delta})^2\mathbf{u} + (\mathbf{\Lambda} - \boldsymbol{\delta})\mathbf{u}^3 + \mathbf{u}^5, \\
\mathbf{a}^{(6)} &= (\mathbf{\Lambda} - \boldsymbol{\delta})^3 + (\mathbf{\Lambda} - \boldsymbol{\delta})^2\mathbf{u}^2 + (\mathbf{\Lambda} - \boldsymbol{\delta})\mathbf{u}^4 + \mathbf{u}^6.
\end{aligned}$$

If we want to recover the Burnett equations via the Chapman-Enskog expansion, the sixth order of  $\mathbf{a}^{(n)}$  is necessary. In this work, we only discuss the equilibrium flow and only the fourth order of the Hermite expansion of the Gaussian distribution is needed

$$G^{(4)} = \rho\omega(\boldsymbol{\xi}) \sum_{n=0}^4 \frac{1}{n!} \mathbf{a}^{(n)} \cdot \mathbf{H}^{(n)}(\boldsymbol{\xi}), \quad (31)$$

where

$$\begin{aligned}
\mathbf{a}^{(0)} \cdot \mathbf{H}^{(0)} &= 1, \\
\mathbf{a}^{(1)} \cdot \mathbf{H}^{(1)} &= u_i \xi_i, \\
\mathbf{a}^{(2)} \cdot \mathbf{H}^{(2)} &= \Lambda_{ij} \xi_i \xi_j - \Lambda_{ii} - \xi^2 + D + (u_i \xi_i)^2 - u^2, \\
\mathbf{a}^{(3)} \cdot \mathbf{H}^{(3)} &= 3\Lambda_{ij} \xi_i \xi_j (u_i \xi_i) \\
&\quad + 3[u^2(\Lambda_{ij} \xi_i \xi_j) + 2(u_i u_j)(\Lambda_{jk} u_j \xi_k)] \\
&\quad + (u_i \xi_i)^3 + 3(u_i \xi_i)^2 \xi^2 - 3(u_i \xi_i)^2 u^2 \\
&\quad - 3(D+2)(u_i \xi_i), \\
\mathbf{a}^{(4)} \cdot \mathbf{H}^{(4)} &= 3\Lambda_{ij} \xi_i \xi_j - 6(\Lambda_{ij} \xi_i \xi_j \\
&\quad + 2\Lambda_{ik} \xi_i \lambda_{jk} \xi_j) + 6(\Lambda_{ii}^2 + 2\Lambda_{ij} \Lambda_{ij}) \\
&\quad + 6\Lambda_{ij} \xi_i \xi_j \xi^2 - 6[(D+4)\Lambda_{ij} \xi_i \xi_j + \Lambda_{ii} \xi^2] \\
&\quad + 6(D+2)\Lambda_{ii} + 6\Lambda_{ij} \xi_i \xi_j (u_k \xi_k)^2 \\
&\quad - 6[\Lambda_{ij} \xi_i \xi_j u^2 + 4\Lambda_{ij} \xi_i u_j (u_k \xi_k) + \Lambda_{ii} (u_k \xi_k)^2] \\
&\quad + 6(\Lambda_{ii} u^2 + \Lambda_{ij} u_i u_j) \\
&\quad + (\xi_i u_i)^4 - 6(\xi_i u_i)^2 u^2 + 3u^4 \\
&\quad - 6[(\xi_i u_i)^2 (u^2 - D - 4) + (D+2 - u^2) \xi^2] \\
&\quad + 3[u^4 - 2(D+2)u^2 + D(D+2)].
\end{aligned}$$

## V. LATTICE BOLTZMANN SCHEME BASED ON THE ES-BGK MODEL

For convenience, we introduced the dimensionless variables,

$$\begin{aligned}
\tilde{\mathbf{x}} &= \frac{\mathbf{x}}{L_0}, & \tilde{\mathbf{u}} &= \frac{\mathbf{u}}{\sqrt{\theta_0}}, & \tilde{\boldsymbol{\xi}} &= \frac{\boldsymbol{\xi}}{\sqrt{\theta_0}}, \\
\tilde{\rho} &= \frac{\rho}{\rho_0}, & \tilde{T}_{eq} &= \frac{T_{eq}}{T_0}, & \tilde{T}_{tr} &= \frac{T_{tr}}{T_0}, \\
\tilde{T}_{rel} &= \frac{T_{rel}}{T_0}, & \tilde{T}_{int} &= \frac{T_{int}}{T_0}, & \tilde{E} &= \frac{E}{\theta_0}, \\
\tilde{e} &= \frac{e}{\theta_0}, & \tilde{e}_{tr} &= \frac{e_{tr}}{\theta_0}, & \tilde{e}_{int} &= \frac{e_{int}}{\theta_0}, \\
\tilde{p} &= \frac{p}{(\rho_0 \theta_0)}, & \tilde{I} &= \frac{I}{\theta_0^{N_f/2}}, & \tilde{G}[g, h] &= \frac{G[g, h] \theta_0^{D/2}}{\rho_0}, \\
\tilde{g} &= \frac{g \theta_0^{D/2}}{\rho_0}, & \tilde{h} &= \frac{h \theta_0^{(D+N_f)/2}}{\rho_0}, & \tilde{\Lambda}_{N_f}^{-1} &= \int \exp(-\tilde{I}^{\frac{2}{N_f}}) d\tilde{I}.
\end{aligned}$$

where  $L_0$  is the characteristic length,  $T_0$  is the characteristic temperature,  $\rho_0$  is the characteristics density,  $t_0$  is the characteristics time, and  $\theta_0 = R_g T_0$ . In the following part, all the variables are dimensionless and the tildes are omitted.

Discretizing  $\boldsymbol{\xi}, g, h, G[g, h]$  in the discrete velocity space, we get  $\boldsymbol{\xi}_i, g_i, h_i$  and  $G_i[g, h]$ . Appendix gives a set of discrete velocity  $\boldsymbol{\xi}_i$  and their corresponding weight  $\omega_i$ . The discrete distribution  $g_i, h_i$  and the Gaussian distribution  $G_i[g, h]$  are defined by

$$g_i = \frac{\omega_i g(\mathbf{x}, \boldsymbol{\xi}_i, t)}{\omega(\boldsymbol{\xi}_i)}, h_i = \frac{\omega_i h(\mathbf{x}, \boldsymbol{\xi}_i, t)}{\omega(\boldsymbol{\xi}_i)}, G_i = \frac{\omega_i G(\mathbf{x}, \boldsymbol{\xi}_i, t)}{\omega(\boldsymbol{\xi}_i)}.$$

Discretizing the evolution equations of  $g$  and  $h$ , i.e., Eq(16) and (18) and inserting the definition of Prandtl number, we obtain the discrete evolution equations of  $g_i$  and  $h_i$ ,

$$\frac{\partial}{\partial t} g_i + \boldsymbol{\xi}_i \cdot \nabla g_i = -\frac{Pr}{\tau} (g_i - G_i[g, h]), \quad (32a)$$

$$\frac{\partial}{\partial t} h_i + \boldsymbol{\xi}_i \cdot \nabla h_i = -\frac{Pr}{\tau} (h_i - \frac{N_f}{2} T_{eq} G_i[g, h]). \quad (32b)$$

In discrete velocity space, the density  $\rho$ , the macroscopic velocity  $\mathbf{u}$  and the specific total energy  $E$  are defined by

$$\rho = \sum_i g_i, \quad (33a)$$

$$\rho \mathbf{u} = \sum_i g_i \boldsymbol{\xi}_i, \quad (33b)$$

$$\rho E = \sum_i g_i \frac{1}{2} \xi_i^2 + \sum_i h_i. \quad (33c)$$

We also have the relationships

$$\rho \left( \frac{1}{2} u^2 + e_{tr} \right) = \sum_i g_i \frac{1}{2} \xi_i^2, \quad (34a)$$

$$\frac{1}{2} \rho e_{int} = \sum_i h_i. \quad (34b)$$

The dimensionless state equation is  $p = \rho T$  and the relationship between the dimensionless temperature  $T_{eq}$ ,

$T_{tr}, T_{int}$  and the corresponding dimensionless energy  $e$ ,  $e_{tr}$ ,  $e_{int}$  are

$$e = \frac{D + N_f}{2} T_{eq}, \quad e_{tr} = \frac{D}{2} T_{tr}, \quad e_{int} = \frac{N_f}{2} T_{int}. \quad (35)$$

The dimensionless correct tensor is

$$\mathbf{\Lambda} = (1 - \kappa)[(1 - \nu)T_{tr}\boldsymbol{\delta} + \nu\boldsymbol{\sigma}] + \kappa T_{eq}\boldsymbol{\delta}. \quad (36)$$

We employ the first order upwind difference scheme to discretize the reduced evolution of  $g$ , i.e. Eq(32a), in space and time

$$g_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) - \frac{Pr}{\tau_f} [g_i(\mathbf{x}, t) - G_i(\mathbf{x}, t)], \quad (37)$$

where  $\Delta t$  is the time step,  $\Delta x$  is the grid step and  $\tau_f = \frac{\tau}{\Delta t}$ . In a similar way, we get the discretized evolution equation of  $h$

$$\begin{aligned} h_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) \\ = h_i(\mathbf{x}, t) - \frac{Pr}{\tau_f} [h_i(\mathbf{x}, t) - \frac{N_f}{2} T G_i(\mathbf{x}, t)]. \end{aligned} \quad (38)$$

From Eq(37) and (38), we can derived the Navier-Stokes equations, with which the Prandtl number is defined by Eq(21) and the specific heat ratio is defined by and (20). Eq(37) and (38) are employed to update the the discrete distribution functions, i.e.  $g_i$  and  $h_i$ .

## VI. NUMERICAL VALIDATION

In this section, the thermal Couette flow and the one dimensional shock tube flow are carried out for verifying the lattice Boltzmann scheme proposed by this work. The lattice model, i.e. D2Q37 given by the Appendix is employed.

### A. Thermal Couette flow

The analytical temperature profile along the  $y$ -direction of the thermal Couette flow is

$$T = T_0 + \frac{Pr}{2Cp} u_0^2 \frac{y}{H} \left(1 - \frac{y}{H}\right) \quad (39)$$

where  $H$  is the distance between the up plate and the down plate,  $y$  is the distance from a point to the down plate,  $u_0$  is the  $x$ -direction velocity of the top plate at the beginning. The dimensionless variables are defined by

$$\tilde{y} = \frac{y}{H}, \quad \tilde{u}_0 = \frac{u_0}{U_0}.$$

Inserting the dimensionless variables  $\tilde{y}, \tilde{u}_0, \tilde{T}$  and the specific heat on constant pressure  $Cp = \frac{D + N_f + 2}{2} R_g$  into

Eq(39), omitting the tildes, the dimensionless analytical solution of the Couette flow is obtained

$$T = 1 + u_0^2 \frac{Pr}{D + N_f + 2} y(1 - y). \quad (40)$$

The specific heat ratio is defined by  $\gamma = \frac{D + N_f + 2}{D + N_f}$ , so  $\gamma$  can be modified by changing  $N_f$ .

We set the initial conditions as  $\rho = 1, T = 1, u_x = u_y = 0$ , where  $u_x$  is the  $x$ -directional velocity and  $u_y$  is the  $y$ -directional velocity. The top plate move with the velocity  $u_0 = 1$  at the beginning. The periodic boundary condition are applied to the left and right sides and the kinetic boundary condition(KBC)[26, 27] are applied to the up and down boundaries. The grid is  $X \times Y = 100 \times 100$ .

Fig(1) shows the simulation result. Here  $\nu$  is  $\nu = 0.5$ ,  $\kappa$  is  $\kappa = 0.2$  and  $N_f$  is  $N_f = 3$ , so the Prandtl number is  $Pr = 0.71$  and the specific heat ratio is  $\gamma = 1.4$ . The numerical solution agrees with the analytical solution very well.

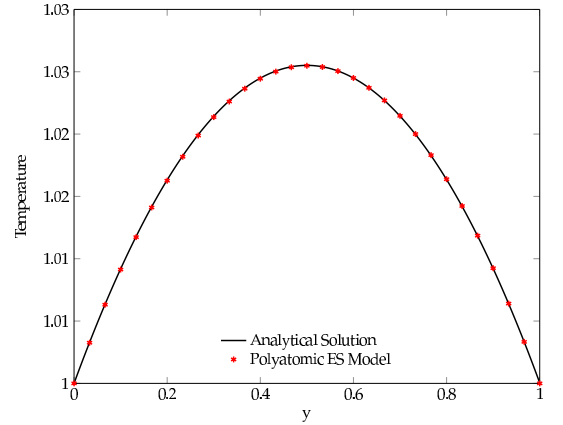


FIG. 1. Thermal Couette flow. The velocity along  $x$  direction of the top plate at the beginning is  $u_0 = 1.0$ , the temperature of the top and the down plate are both  $T_0 = 1.0$ . The parameters are defined by  $\nu = 0.5$ ,  $\kappa = 0.2$  and  $N_f = 3$ . The Prandtl number is  $Pr = 0.71$  and the specific heat ratio is  $\gamma = 1.4$

### B. The Shock tube flow of 1D

The shock tube problem of one dimension has been discussed intensively[28]. Here, the initial condition is given by

$$\begin{aligned} (\rho_L, T_L, u_{Lx}) &= (4, 1, 0) \\ (\rho_R, T_R, u_{Rx}) &= (1, 1, 0) \end{aligned}$$

where the subscript  $L$  indicates the left side of the shock tube and  $R$  indicates the right side of the shock tube.  $u_x$  is the macroscopic velocity along the  $x$  coordinate.

We set the specific heat ratio as  $\gamma = 1.4$  and the relaxation time as  $\tau = 2/3$ . The grid is  $X \times Y = 1000 \times 16$ . The additional degrees is  $N_f = 3$ . The periodic boundary

condition is employed for the up and down boundaries and the open boundary condition is performed for the left and right boundaries.

Fig(2) shows the simulation results at *step* 180, i.e. at the time

$$t = \frac{\text{step}}{X \times r} = \frac{180}{1000 \times 1.1969797752} = 0.1504.$$

It can be seen that the simulation results agree with the analytical resolutions well.

## VII. CONCLUSION

A lattice Boltzmann scheme based on the polyatomic ES-BGK is proposed, from which the Navier-Stokes equations associated with flexible Prandtl number and specific heat ratio are derived via the Chapman-Enskog expansion. As the scheme proposed is based on the polyatomic ES-BGK model, it has solid physical basis. The Gaussian distribution is expanded on the Hermite polynomials and the general term formula for the Hermite coefficients of the Gaussian distribution is deduced. This is the key point of the scheme proposed. The thermal Couette flow and the shock tube flow of one dimension are performed to verify the scheme given by this work. The simulation results agree with the analytical resolutions excellently. The scheme proposed gives a new way to modify

the Prandtl number and the specific heat ratio in the LBM.

## Appendix A: LB models of 2D

Employing the Hermite quadrature, which has been intensively discussed in [25, 29, 30], [31, 32], [33, 34], we construct a 2D LB model, i.e. D2Q37. The model proposed are of fourth-order accuracy. The discrete particle velocity sets and the weights  $\omega_i$  of D2Q37 are showed in Table(I).

TABLE I. Discrete velocities and weights of D2Q37. Perm denotes permutation and  $k$  denotes the number of discrete velocities included in each group. Scaling factor is  $r = 1.19697977$ .

$k$	$\xi_i$	$\omega_i$
1	(0, 0)	$2.03916918e-1$
4	$Perm(r, 0)$	$1.27544846e-1$
4	$Perm(r, r)$	$4.37537182e-2$
4	$Perm(2r, 0)$	$8.13659044e-3$
4	$Perm(2r, r)$	$9.40079914e-3$
4	$Perm(3r, 0)$	$6.95051049e-4$
4	$Perm(3r, r)$	$3.04298494e-5$
4	$Perm(3r, 3r)$	$2.81093762e-5$

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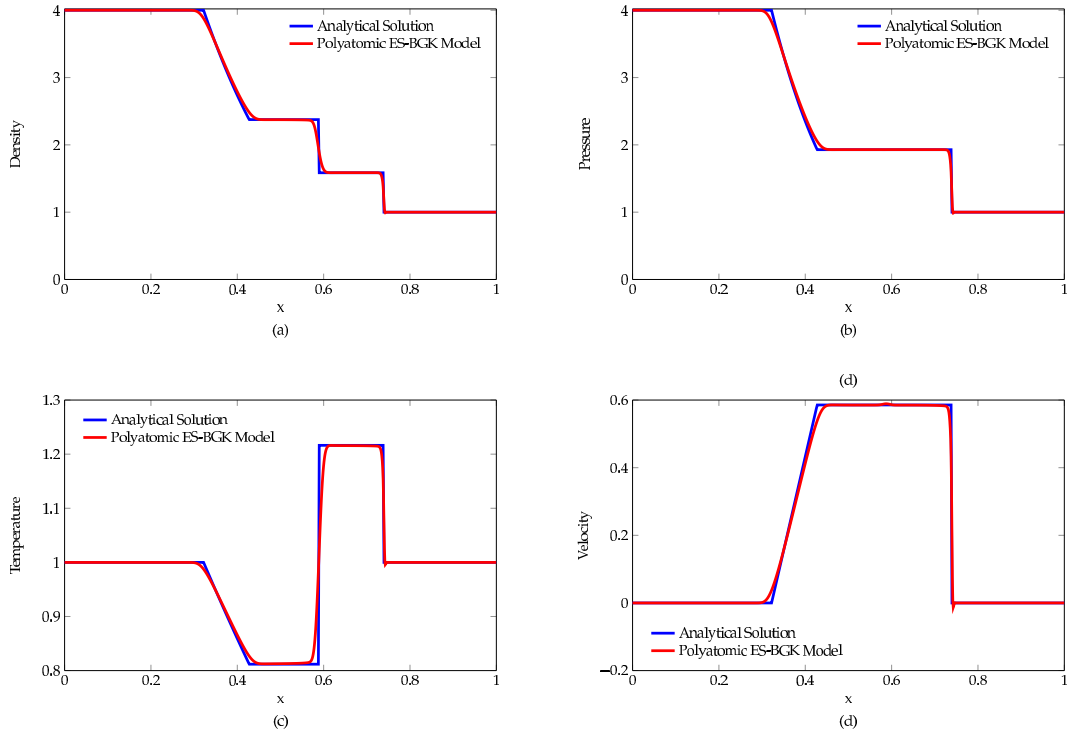


FIG. 2. The simulation results of D2Q37 and the analytical resolutions at the time  $t=0.1504$ . The specific heat ratio is  $\gamma=1.4$  and the parameter  $N_f$  is 3. The relaxation time is  $\tau=2/3$ . The initial condition of the left side is  $\rho=4, T=1, \mathbf{u}=0$  and that of the right side is  $\rho=1, T=1, \mathbf{u}=0$ .

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